



chain nodes :

7 8 9 10 11 12 13 14 15 22 23 24 25 26 27 28 29 30

ring nodes :

1 2 3 4 5 6 16 17 18 19 20 21 31 32 33 34 35 36

chain bonds :

1-9 2-7 7-8 9-10 9-11 10-14 10-15 11-12 12-13 16-24 17-22 22-23 23-31 24-25 24-26
25-29 25-30 26-27 27-28

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 31-32 31-36 32-33
33-34 34-35 35-36

exact/norm bonds :

9-11 10-15 11-12 12-13 22-23 23-31 24-26 25-30 26-27 27-28

exact bonds :

1-9 2-7 7-8 9-10 10-14 16-24 17-22 24-25 25-29

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21 31-32 31-36 32-33
33-34 34-35 35-36

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS
31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom